

POSETTED TREES AND BAKER-CAMPBELL-HAUSDORFF PRODUCT

DONATELLA IACONO AND MARCO MANETTI

ABSTRACT. We introduce the combinatorial notion of posetted trees and we use it in order to write an explicit expression of the Baker-Campbell-Hausdorff formula.

1. INTRODUCTION

If a, b are continuous operators on a Hilbert space, we may write

$$e^a e^b = e^{a \bullet b}, \quad a \bullet b = a + b + \sum_{n=2}^{\infty} w_n(a, b),$$

where w_n is a universal, non commutative, homogeneous polynomial of degree n with rational coefficients. The product \bullet is called, after [1, 2, 8], Baker-Campbell-Hausdorff (BCH) product: it is associative and the BCH theorem asserts that every polynomial w_n is a Lie element, i.e., is a linear combination of nested commutators. However, the proof of the BCH theorem does not give directly an explicit description of w_n as a Lie element; moreover, such description is not unique in view of the Jacobi identity.

The most famous explicit expression of $a \bullet b$, in terms of nested commutators, is probably the one due to E. Dynkin (see [4, Equation 1] or [3, Equation 1.7.3]):

$$(1) \quad a \bullet b = \sum_{n \geq 0} \frac{(-1)^{n-1}}{n} \sum \frac{1}{p_1! q_1! \dots p_n! q_n!} ad(a)^{p_1} ad(b)^{q_1} \dots ad(a)^{p_n} ad(b)^{q_n-1} b,$$

where $ad(x) = [x, -]$ is the adjoint operator, the second sum is over all possible combinations of $p_1, q_1, \dots, p_k, q_k \in \mathbb{N}$ such that $p_i + q_i > 0$, for $i = 1, \dots, k$, and $\sum_{i=1}^k (p_i + q_i) = n$.

The literature about Baker-Campbell-Hausdorff formula is huge. For instance: in 1998, V. Kathotia [9] derived a trees summation expression for the BCH product over the real numbers using M. Kontsevich's universal formula for deformation quantization of Poisson manifolds; the coefficient of this formula are certain integrals on configuration spaces and it is still unknown if they are rational numbers. In the papers [5] and [6], the authors recognize the equation $a \bullet b \bullet c = 0$ as the Maurer-Cartan equation of the canonical L_∞ structure on the conormalized complex of singular cochains, on the standard two dimensional simplex with values in a Lie algebra. Therefore, the possibility of an explicit description of $a \bullet b$, again as a trees summation formula, by using the standard tools of homological perturbation and homotopy transfer theory [11]. The reader may also consult [16] for a list of explicit and recursive formulas.

The aim of this paper is to give a simple and elementary combinatorial description of the polynomial w_n that uses some notions about planar rooted trees. The necessary combinatorial background is summarized in Sections 2 and 3. In particular, for every finite planar rooted tree Γ , the set of its leaves admits a total ordering (from left to right) and also a partial ordering \preceq , which takes care of the position of leaves with respect to the subroots. Then, we define a posetted tree as a finite planar rooted tree, whose leaves are labelled by elements on a partially ordered set (a poset), monotonically with respect to \preceq .

Our main result (Theorem 11) gives an explicit description of every w_n as a linear combination with rational coefficients of nested commutators, indexed by a certain set of posetted trees with n leaves. The

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formula of the coefficients involves the Bernoulli numbers and is completely described in terms of the combinatorial data of posetted trees.

2. SUBROOTS OF PLANAR ROOTED TREES

This section is devoted to introduce the notion, already known in the parallel logic programming community [14], of subroots of a planar rooted trees.

Recall that a tree is called a *rooted tree* if one vertex has been designated the *root*. Every rooted tree has a natural structure of directed tree such that, for every vertex u , there exists a unique directed path from u to the root. We shall write $u \rightarrow v$ if the vertex v belongs to the directed path from u to the root. A *leaf* is a vertex without incoming edges: equivalently, a vertex u is a leaf if the relation $v \rightarrow u$ implies $u = v$. A vertex is called *internal* if it is not a leaf; notice that, if a rooted tree has at least two vertices, then the root is an internal vertex.

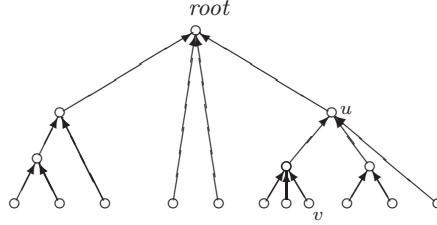


FIGURE 1. A rooted tree, with $v \rightarrow u$.

From now on, we consider only planar rooted trees; following [12], we denote by \mathcal{T} the set of finite planar rooted trees with the root at the top and the leaves at the bottom (i.e., every directed path moves upward), and such that every internal vertex has at least two incoming edges.

We also write

$$\mathcal{T} = \bigcup_{n \geq 0} \mathcal{T}_n,$$

where \mathcal{T}_n is the set of planar rooted trees with n leaves and, for every $\Gamma \in \mathcal{T}$, we denote by $L(\Gamma)$ the set of leaves of Γ . The planarity of the tree gives, for every internal vertex v , a total ordering of the edges ending in v , from the leftmost to the rightmost (see Figure 2).

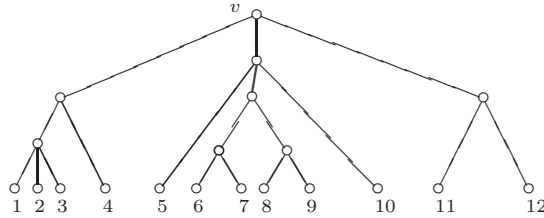
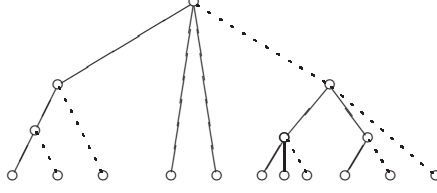


FIGURE 2. An element of \mathcal{T}_{12} .

Definition 1. A *rightmost branch* of a planar rooted tree $\Gamma \in \mathcal{T}$ is a maximal connected subgraph $\Omega \subset \Gamma$, with the property that every edge of Ω is a rightmost edge of Γ . A rightmost branch is called non trivial if it has at least two vertices.


 FIGURE 3. An element of \mathcal{T}_{11} . The dashed lines denote the rightmost edges.

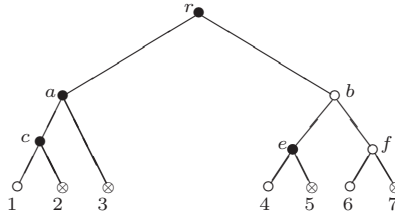
Definition 2. A *local rightmost leaf* is a leaf lying on a non trivial rightmost branch. Given an internal vertex v , we call $m(v)$ the leaf lying on the rightmost branch containing v . We also denote by $d(v)$ the distance between v and $m(v)$, as defined in [13].

Definition 3. A *subroot* is the vertex of a non trivial rightmost branch which is nearest to the root. The set of subroots of a finite planar rooted tree Γ will be denoted by $R(\Gamma)$.

Therefore, we have the natural bijections

$$\{ \text{subroots} \} \cong \{ \text{non trivial rightmost branches} \} \cong \{ \text{local rightmost leaves} \}.$$

Example 4. In the tree of Figure 4, the subroots are the vertices r, a, c and e ; the rightmost leaves are the leaves 2, 3, 5 and 7. Moreover, $m(a) = 3, m(c) = 2, m(e) = 5$ and $m(r) = m(b) = m(f) = 7$; and $d(r) = 3, d(b) = 2$ and $d(a) = d(c) = d(e) = d(f) = 1$.


 FIGURE 4. The subroots are denoted by \bullet , while the local rightmost leaves by \otimes .

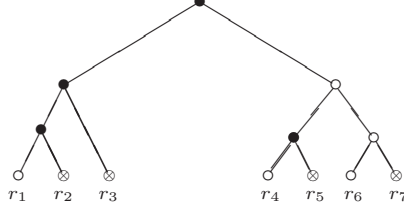
A planar rooted tree $\Gamma \in \mathcal{T}$ is a *binary tree* if every internal vertex has exactly two incoming edges. We use the notation

$$\mathcal{B} = \bigcup_{n \geq 0} \mathcal{B}_n \subset \mathcal{T},$$

where \mathcal{B}_n is the set of planar binary rooted trees with n leaves. Using the notion introduced above, it is very easy to see that a tree $\Gamma \in \mathcal{T}_n$ is a binary tree if and only if it satisfies the equality:

$$\sum_{v \in R(\Gamma)} d(v) = n - 1.$$

Let R be a (non associative) algebra over a field \mathbb{K} and $\Gamma \in \mathcal{B}$ a planar rooted tree. Labelling the leaves of Γ with elements of R , we can associate the product element in R obtained by the usual operadic rules [11, 12], i.e., we perform the product of R at every internal vertex in the order arising from the planar structure of the directed tree. For instance, the following labelled tree



gives the product $((r_1 r_2) r_3)((r_4 r_5)(r_6 r_7)) \in R$.

Given any map $f : L(\Gamma) \rightarrow R$ (the labelling), we denote by $Z_\Gamma(f) \in R$ the corresponding product element.

If $S \subset R$, then the elements $Z_\Gamma(f)$, with $\Gamma \in \mathcal{B}$ and $f : L(\Gamma) \rightarrow S$, are a set of generators of the subalgebra generated by S . If R is either symmetric or skewsymmetric (e.g., a Lie algebra), then we may reduce the set of generators by a suitable choice of the labelling. Keeping in mind our main application (the BCH product), a possible way of doing that is by introducing the combinatorial notion of posetted trees.

3. POSETTED TREES

Using the notion of subroot, we can define a partial order \preceq on the set of leaves $L(\Gamma)$.

Definition 5. Given two leaves l_1 and l_2 in a tree $\Gamma \in \mathcal{T}$, we say $l_1 \preceq l_2$ if $l_1 = l_2$ or there exists a subroot $v \in R(\Gamma)$ such that $l_2 = m(v)$ and $l_1 \rightarrow v$.

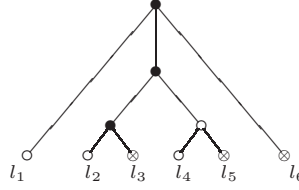


FIGURE 5. Here, we have $l_1 \preceq l_6$, $l_2 \preceq l_3 \preceq l_5 \preceq l_6$ and $l_4 \preceq l_5$.

Definition 6. For every poset (A, \leq) , we denote

$$\mathcal{T}(A) = \{(\Gamma, f) \mid \Gamma \in \mathcal{T}, f : (L(\Gamma), \preceq) \rightarrow (A, \leq), f \text{ monotone}\}$$

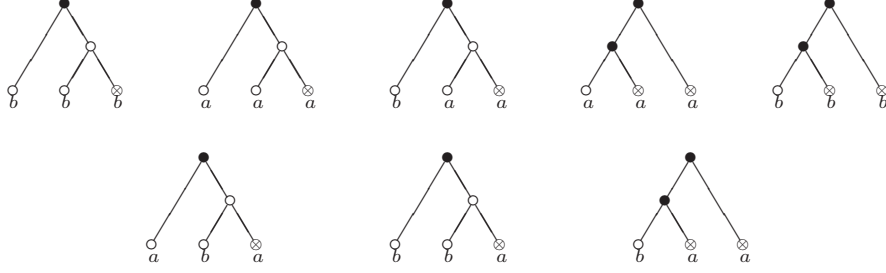
In a similar way, we define $\mathcal{B}(A)$, and, for every $n > 0$, $\mathcal{T}_n(A)$ and $\mathcal{B}_n(A)$.

We call *posetted trees* the elements of $\mathcal{T}(A)$.

Example 7. The sets $\mathcal{B}_1(b \leq a)$, $\mathcal{B}_2(b \leq a)$ and $\mathcal{B}_3(b \leq a)$ contain 2, 3 and 8 posetted trees, respectively (see Figures 6 and 7).



FIGURE 6. The 5 posetted trees of $\mathcal{B}_i(b \leq a)$, $i = 1, 2$.


 FIGURE 7. The 8 posetted trees of $\mathcal{B}_3(b \leq a)$.

Remark 8. If $A = \{1, \dots, m\}$ with the usual order, then there exists a natural inclusion of $\mathcal{T}_n(A)$ into the set of admissible graphs with n vertices of the first kind and m vertices of the second kind considered in [9, 10].

Assume that A is a subset of a (skew)commutative algebra R and choose a total ordering on A . Then, it is easy to see that the elements $Z_\Gamma(f)$, with $(\Gamma, f) \in \mathcal{B}(A)$ generate, as a \mathbb{K} vector space, the subalgebra generated by A .

4. AN EXPRESSION OF THE BAKER-CAMPBELL-HAUSDORFF PRODUCT IN TERMS OF POSETTED TREES

Let L be a Lie algebra over a field \mathbb{K} of characteristic 0, which is complete with respect to its lower descending series $L^1 = L$, $L^{n+1} = [L^n, L]$. Denote by $\bullet: L \times L \rightarrow L$ the Baker-Campbell-Hausdorff (BCH) product, obtained formally by the formula $a \bullet b = \log(e^a e^b)$. It is well known that

$$a \bullet b = a + b + \frac{1}{2}[a, b] + \frac{1}{12}[a, [a, b]] - \frac{1}{12}[b, [b, a]] + \dots,$$

is an element of the Lie subalgebra generated by a and b and, then, it can be expressed as an infinite sum

$$a \bullet b = \sum_{(\Gamma, f) \in \mathcal{B}(b \leq a)} s_{(\Gamma, f)} Z_\Gamma(f),$$

for a sequence $s_{(\Gamma, f)} \in \mathbb{K}$. Clearly, in view of the alternating properties of the product and Jacobi identity, such a sequence is not unique. The Dynkin Formula (1) provides a sequence as above where $s_{(\Gamma, f)} = 0$, whenever Γ has at least 2 subroots: on the other hand, the explicit expression of the nonvanishing $s_{(\Gamma, f)}$ is rather complicated.

Here, we describe another sequence $b_{(\Gamma, f)}$ of rational numbers with the above properties. First of all, define the sequence of rational numbers $\{b_n\}$, for every $n \geq 0$, by their ordinary generating function

$$\sum_{n \geq 0} b_n x^n = \frac{x}{e^x - 1}.$$

Notice that $b_n = B_n n!$ where the B_n are the Bernoulli numbers. In particular, the only non trivial odd term of the sequence is $b_1 = -\frac{1}{2}$ and we have:

$$b_0 = 1, \quad b_2 = \frac{1}{12}, \quad b_4 = -\frac{1}{720}, \quad \dots$$

Definition 9. Given a poset A and a posetted tree $(\Gamma, f) \in \mathcal{T}(A)$, let us define

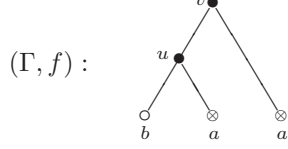
$$b_{(\Gamma, f)} := \prod_{v \in R(\Gamma)} \frac{b_{d(v)}}{t(v)},$$

where the b_n 's are the rational numbers above and, for every subroot $v \in R(\Gamma)$, we have

$$t(v) = \text{number of leaves } u \in L(\Gamma) \text{ such that } u \rightarrow v \text{ and } f(u) = f(m(v)).$$

We remind that $m(v)$ is the leaf lying on the rightmost branch containing v (Definition 2).

Example 10. Let $A = \{b \leq a\}$ and consider the posetted tree



Here, we have $d(u) = d(v) = 1$; $t(u) = 1$; $t(v) = 2$; therefore, $b_{(\Gamma, f)} = \frac{b_1}{1} \cdot \frac{b_1}{2} = \frac{1}{8}$.

Theorem 11. Let L be a Lie algebra as above; then, for every positive integer k and every $a_1, \dots, a_k \in L$, we have

$$(2) \quad a_k \bullet a_{k-1} \bullet \dots \bullet a_1 = \sum_{(\Gamma, f) \in \mathcal{B}(a_1 \leq a_2 \leq \dots \leq a_k)} b_{(\Gamma, f)} Z_{\Gamma}(f),$$

$$(3) \quad a_1 \bullet a_2 \bullet \dots \bullet a_k = \sum_{n=1}^{+\infty} (-1)^{n-1} \sum_{(\Gamma, f) \in \mathcal{B}_n(a_1 \leq a_2 \leq \dots \leq a_k)} b_{(\Gamma, f)} Z_{\Gamma}(f).$$

In particular, for $a, b \in L$, we have

$$(4) \quad a \bullet b = \sum_{(\Gamma, f) \in \mathcal{B}(b \leq a)} b_{(\Gamma, f)} Z_{\Gamma}(f).$$

Proof. Let us first prove Formula (4). Let $\mathcal{C}'(b \leq a) \subset \mathcal{B}(b \leq a)$ be the subset of posetted trees having every local rightmost leaf labelled with a and denote by $\mathcal{C}(b \leq a) = \mathcal{C}'(b \leq a) \cup \mathcal{B}_1(b)$.

Since the bracket is skewsymmetric, we have that $Z_{\Gamma}(f) = 0$, for every $(\Gamma, f) \notin \mathcal{C}(b \leq a)$; therefore,

$$\sum_{(\Gamma, f) \in \mathcal{B}(b \leq a)} b_{(\Gamma, f)} Z_{\Gamma}(f) = \sum_{(\Gamma, f) \in \mathcal{C}(b \leq a)} b_{(\Gamma, f)} Z_{\Gamma}(f).$$

In [3, Theorem. 1.6.1] and [7], the following recursive formula for the Baker-Campbell-Hausdorff product is proved:

$$a \bullet b = \sum_{r \geq 0} Z_r,$$

where

$$Z_0 = b, \quad Z_{r+1} = \frac{1}{r+1} \sum_{m \geq 0} b_m \sum_{i_1 + \dots + i_m = r} (\text{ad } Z_{i_1})(\text{ad } Z_{i_2}) \dots (\text{ad } Z_{i_m})a, \quad \text{for } r \geq 0.$$

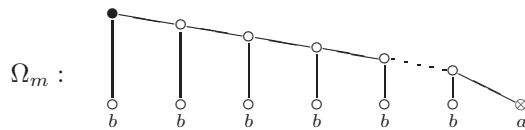
For every $r > 0$, let $\mathcal{C}_r \subset \mathcal{C}(b \leq a)$ be the subset of posetted trees with exactly r leaves labelled with a ; we prove that, for every $r \geq 0$, we have

$$(5) \quad Z_r = \sum_{(\Gamma, f) \in \mathcal{C}_r} b_{(\Gamma, f)} Z_{\Gamma}(f).$$

This is clear for $r = 0$; for $r = 1$, we have

$$Z_1 = \sum_{m \geq 0} b_m (\text{ad } Z_0)^m a = \sum_{m \geq 0} b_m (\text{ad } b)^m a,$$

whereas $\mathcal{C}_1 = \{\Omega_m\}$, $m \geq 0$, is the set of posetted trees of Bernoulli type [15], i.e.,



where m is the number of leaves labelled with b . Therefore, the coefficient $b_{(\Omega_m)}$ is exactly b_m and so

$$Z_1 = \sum_{(\Gamma, f) \in \mathcal{C}_1} b_{(\Gamma, f)} Z_\Gamma(f).$$

Moreover, every element of \mathcal{C}_{r+1} is obtained in a unique way starting from a tree Ω_m and grafting, at each of the m leaves labelled with b , the roots of elements of $\mathcal{C}_{i_1}, \dots, \mathcal{C}_{i_m}$, with $i_1 + \dots + i_m = r$ (for the definition of the grafting see [12, Definition 1.37]). Therefore, the proof of (5) follows easily by induction on r .

Next, since \bullet is associative, we have

$$a_1 \bullet a_2 \bullet \dots \bullet a_k = -((-a_k) \bullet \dots \bullet (-a_1)),$$

and Formula (3) follows immediately from (2). Finally, setting $b = a_{k-1} \bullet \dots \bullet a_1$, we have that every posetted tree of $\mathcal{B}(a_1 \leq a_2 \leq \dots \leq a_k)$ can be described in a unique way as a posetted tree in $\mathcal{C}(b \leq a_k)$, where at every leaf labelled with b is grafted the root of a posetted tree of $\mathcal{B}(a_1 \leq a_2 \leq \dots \leq a_{k-1})$. In view of the associativity relation

$$a_k \bullet a_{k-1} \bullet \dots \bullet a_1 = a_k \bullet b,$$

we obtain that (2) is a consequence of $a_k \bullet b = \sum_{(\Gamma, f) \in \mathcal{C}(b \leq a_k)} b_{(\Gamma, f)} Z_\Gamma(f)$.

□

Remark 12. Choose $a_1 = b$ and $a_2 = a$ in Equation (2), and $a_1 = a$ and $a_2 = b$ in Equation (3). Comparing the coefficient of the product $ad(b)^n(a)$ in both equations, we obtain the following relations

$$(6) \quad (1 + n(-1)^n)b_n = - \sum_{i=1}^{n-1} (-1)^i b_i b_{n-i}, \quad n > 0.$$

Indeed, the coefficient of $ad(b)^n(a)$ in Equation (3) comes from the Bernoulli tree Ω_n and so it is exactly b_n . On the other side, we need to consider the subset $S(n)$ of trees $(\Gamma, f) \in \mathcal{B}(a \leq b)$ with only one subroot, n leaves labelled b and one leaf labelled a . For any $(\Gamma, f) \in S(n)$, we have $Z_\Gamma(f) = \pm ad(b)^n(a)$, and we can define C_n as

$$\sum_{(\Gamma, f) \in S(n)} b_{(\Gamma, f)} Z_\Gamma(f) = C_n ad(b)^n(a).$$

Comparing the coefficients, we have

$$C_n = (-1)^n b_n.$$

Next, let us compute C_n recursively. There are two different types of contributions to C_n due to the following graphs. The first contribution is due to the graph with only one subroot; in this case, the coefficient is $\frac{b_n}{n} ad(b)^{n-1}([a, b]) = -\frac{b_n}{n} ad(b)^n(a)$. The other contribution is due to the graphs obtained from a graph in $S(i)$, for every $i = 1, \dots, n-1$, and grafting, at the leaves labelled with a , a graph of $S(n-i)$. Therefore, for every fixed i , the coefficient is

$$\frac{b_i}{n} C_{n-i} ad(b)^{i-1}([ad(b)^{n-i}(a), b]) = -\frac{b_i}{n} C_{n-i} ad(b)^n(a).$$

Summing up, we have

$$C_n = -\frac{b_n}{n} - \sum_{i=1}^{n-1} \frac{b_i}{n} C_{n-i};$$

and, since $C_n = (-1)^n b_n$, we get the relation

$$b_n(1 + n(-1)^n) = - \sum_{i=1}^{n-1} (-1)^i b_i b_{n-i}.$$

Note that, in the previous computation, we have just used the fact that the product is associative and therefore apply for every associative product defined by Equation (2). More precisely, let a_n be any sequence in \mathbb{K} , and for any $(\Gamma, f) \in \mathcal{B}(b \leq a)$, define

$$a_{(\Gamma, f)} := \prod_{v \in R(\Gamma)} \frac{a_{d(v)}}{t(v)},$$

and the product

$$(7) \quad a * b = \sum_{(\Gamma, f) \in \mathcal{B}(b \leq a)} a_{(\Gamma, f)} Z_{\Gamma}(f).$$

Proposition 13. *In the notation above, the product $*$ is associative if and only if there exists an $h \in \mathbb{K}$ such that $a_n = h^n b_n$, for every $n > 0$.*

Proof. One implication is clear, if $a_n = h^n b_n$, then

$$a * b = \sum_{(\Gamma, f) \in \mathcal{B}(b \leq a)} a_{(\Gamma, f)} Z_{\Gamma}(f) = \sum_{(\Gamma, f)} \prod_{v \in R(\Gamma)} h^{d(v)} b_{(\Gamma, f)} Z_{\Gamma}(f) = h^{-1}((ha) \bullet (hb));$$

this implies that the product $*$ is associative (in the last equality we use that $\sum_{v \in R(\Gamma)} d(v) = n - 1$). As regards the other implication, assume that the product $*$ is associative; then, Equation (3) holds for the product $*$ instead of \bullet . Arguing as in the above remark, we conclude that the numbers a_n must satisfy Equation (6), and this easily implies that $a_n = (-2a_1)^n b_n$, for every $n > 0$. □

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UNIVERSITÀ DEGLI STUDI DI BARI,
DIPARTIMENTO DI MATEMATICA,
VIA E. ORABONA 4, I-70125 BARI, ITALY.

E-mail address: `iacono@dm.uniba.it`

URL: `www.dm.uniba.it/~iacono/`

UNIVERSITÀ DEGLI STUDI DI ROMA “LA SAPIENZA”,
DIPARTIMENTO DI MATEMATICA “GUIDO CASTELNUOVO”,
P.LE ALDO MORO 5, I-00185 ROMA, ITALY.

E-mail address: `manetti@mat.uniroma1.it`

URL: `www.mat.uniroma1.it/people/manetti/`